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In recent years, Process Intensification (PI) has attracted considerable interest as a potential means of process improvements and to meet the increasing demands for sustainable production. PI aims to improve processes by increasing efficiency, reducing energy consumption, operational costs, volume, and waste as well as simplifying the flowsheet. A variety of intensified operations and equipment has been developed. Potentially, this creates a large number of options for possible process improvement, however, to date only a limited number of intensified technologies have achieved implementation, such as reactive distillation, dividing wall columns and reverse flow reactors [1]. One major reason for this is that the identification of the best PI option is neither simple nor systematic.

In previous work [2] we reported the development of a general computer-aided systematic synthesis and design methodology in which redundant intensified options are systematically removed by checking against predefined constraints through a decomposition approach of a superstructure optimization problem. In this approach lower level steps employ simple and easy calculations, while the higher level steps employ more rigorous and detailed calculations. However, up to now, this methodology is limited to already reported PI unit operations which can be retrieved, together with all information necessary for synthesis and design of each of them, from a knowledge base tool. In order to invent new unit operations going beyond those currently in existence, process synthesis and design incorporating PI needs to be investigated at the phenomenological level [3, 4] which will be presented in this contribution. The basis of the phenomena-based process synthesis is transfer units consisting of mass, component, energy and momentum balances as well as phenomena building blocks and model equations describing them. Following the same rationale as the general methodology described previously, the problem is first defined, given a set of product quality and quantity as well as additional process constraints in addition to the potential need for the improvement. Next, the given information is analyzed to identify all potential phenomena building blocks. In the next step, the phenomena building blocks are joined together according to combination rules to match process intensification targets defined through a superstructure of flowsheet options. Based on these, the generated options are screened through performance specifications before unit operations are identified. For example, a counter-current sequence of similar simultaneous mixing and vapour-liquid phenomena with the final steps at both ends being simultaneous heat transfer, mixing and vapour-liquid phase change phenomena can be identified as a distillation column. In the penultimate step, the remaining options are optimized with respect to a defined objective function. The results are verified through rigorous model simulations in the final step. The advantage of the phenomena-based process synthesis and design is that it generates potentially novel process options because the initial search space is wider than the search space of existing units (truly predictive models lead to reliable predictive solutions) as well as the simultaneous development of the necessary process models.

In this contribution the application of a phenomena-based process synthesis combined with a systematic methodology through a computer-aided framework will be described and highlighted with selected examples in the area of distillation systems, together with a focus on some of the suitable methods and tools.

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